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Bias induced strain in AlGaN/GaN heterojunction field effect transistors and its implications

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We report gate bias dependence of the charge due to piezoelectric polarization obtained by using a fully coupled formulation based upon the piezoelectric constitutive equations for stress and electric displacement. This formulation is significant because it fully accounts for electromechanical coupling under the constraint of global charge control. The coupled formulation results in lower charge due to piezoelectric polarization as compared to the uncoupled formulation for a given Al mole fraction. With increasing two dimensional electron gas concentration, that is, for gate biases greater than threshold, the compressive strain along the *c* axis in the barrier AlGaN layer increases with a concomitant increase of in-plane stress. Current collapse is correlated to the increase in source and drain resistances through their dependence upon surface charge. An alternate explanation of current collapse using local charge neutrality is also presented. [DOI: 10.1063/1.2203739]

GaN-based heterojunction field effect transistors (HFETs) are currently being vigorously pursued for possible applications in high temperature and high power environment. Devices have been fabricated with superb power performance, notably the recently reported 12 W/mm at 10 GHz with a GaN/AlGaN/GaN high electron mobility transistor (HEMT) without surface passivation.[1] Further enhancement and optimization of device performance may be possible with a clearer understanding of the underlying physics of GaN-based HFETs. In this letter, we investigate the gate bias dependence of piezoelectric polarization and its possible implications on GaN-based device performance.

The presence of spontaneous polarization and strain induced polarization in AlGaN/GaN HFETs has been widely recognized. The basic HFET material structure consists of a thick GaN layer on which is grown a pseudomorphic AlGaN layer. Both GaN and AlGaN are grown in the hexagonal wurtzite crystal structure with the *c* axis normal to the interface. For purposes of analysis, the layers are usually assumed to be of infinite extent in the *c* plane, the *c*-plane lattice constant of the pseudomorphic AlGaN is assumed clamped at the lattice constant of the GaN layer, and shear stresses are assumed absent. Because the bulk *c*-plane lattice constant of AlN, 3.112 Å, is smaller than that of bulk GaN, 3.189 Å, the clamped AlGaN lattice results in tensile stress and strain in the *c* plane and compressive strain along the *c* axis which is assumed to be stress free. Following the method used for weakly piezoelectric materials, most analyses use these assumptions to compute the *c*-plane stresses and *c*-axis strain from the tensor formulation of Hooke's law, and then compute the piezoelectric polarization charge from the stress or strain components using the piezoelectric moduli. The piezoelectric polarization is then added to the fixed spontaneous polarization to perform further analysis of the HFET operation.[2–4] With both AlGaN and GaN being rather strong piezoelectric materials a more complete approach would use fully coupled electromechanical equations to relate stress to the electric field as well as to the strain in these systems.[5] In this letter, we apply the fully coupled equations to the AlGaN/GaN HFET. The coupled formulation results in piezoelectric polarization charge that is 6.0% lower than the simplified uncoupled model for the technologically important $Al_{0.3}Ga_{0.7}Al$/GaN structure.

The coupled formulation is based on the linear piezoelectric constitutive equations for stress and electric displacement,[6]

$$\begin{aligned} \sigma_{ij} &= C_{ijkl}\varepsilon_{kl} - e_{kij}E_k, \\ D_i &= e_{ijk}\varepsilon_{jk} - \kappa_{ij}E_j + P_i^S, \end{aligned} \tag{1}$$

where σ_{ij} is the stress tensor, C_{ijkl} is the fourth rank elastic stiffness tensor, ε_{kl} is the strain tensor, e_{ijk} is the third ranked piezoelectric coefficient tensor, κ_{ij} is the second rank permittivity tensor, D_i is the electric displacement, E_k is the electric field, and P_i^s is the spontaneous polarization. The indices i, j, k, and l run over the Cartesian coordinates 1, 2, and 3 (x, y, and z). Einstein's rule of summation over repeated indices is implied. The symmetry of the wurtzite crystal structure of GaN and AlGaN reduces the number of independent elastic and piezoelectric moduli. In the devices considered here, the crystals are grown with the c axis normal to the surface in the z direction, we make the common assumption that the thick GaN layer is unstrained and the biaxial strain of the thin AlGaN layer satisfies $\varepsilon_x = \varepsilon_y = (a_{GaN} - a_{AlGaN})/a_{AlGaN}$, where a_{GaN} and a_{AlGaN} are the c-plane lattice constants of each material. The absence of stress along the growth direc-

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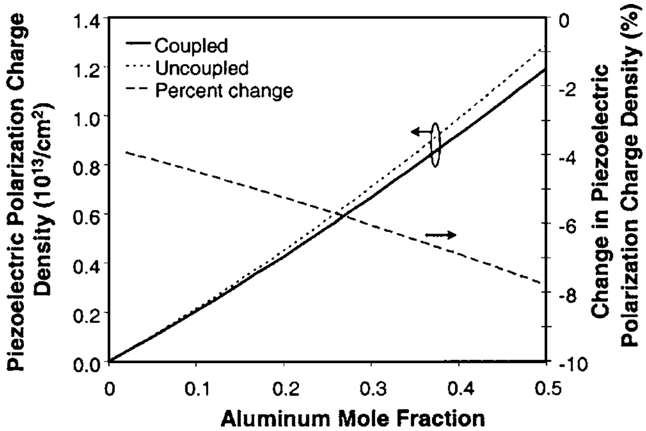

FIG. 1. Charge due to piezoelectric polarization as a function of aluminum mole fraction for a pseudomorphic AlGaN layer on GaN.

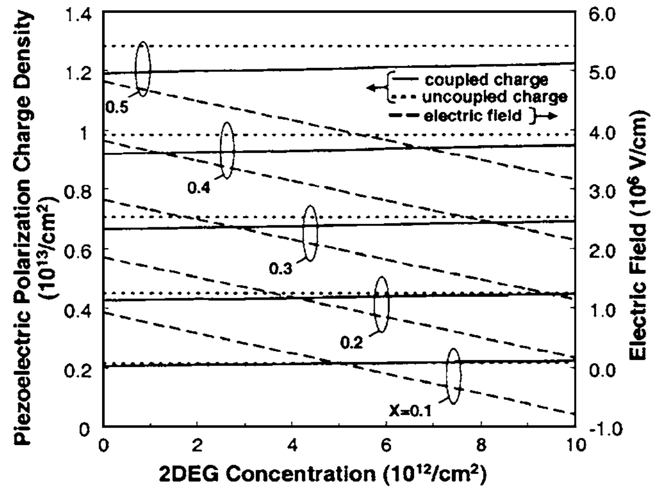

FIG. 2. Piezoelectric charge component for a pseudomorphic $Al_xGa_{1-x}N$ layer on GaN as a function of the 2DEG concentration with aluminum mole fraction, x, as a parameter. The solid lines represent the variation of piezoelectric charge density using the modified formulation and dotted lines show the uncoupled charge density. Dashed lines show the corresponding electric field in fully coupled case.

tion (z direction), in the barrier AlGaN layer, allows us to express the strain along the growth direction as

$$\varepsilon_z = -2\frac{C_{13}}{C_{33}}\varepsilon_x + \frac{e_{33}}{C_{33}}E_z^{\mathrm{AlGaN}}. \tag{2}$$

where E_z^{AlGaN} is the z-directed electric field in the barrier AlGaN layer and we have expressed the elastic and piezoelectric moduli in matrix notation.[7]

The areal charge concentration due to piezoelectric polarization in AlGaN is expressed as follows:

$$P_{\mathrm{PE}}^{\mathrm{AlGaN}} = 2\varepsilon_x\left(e_{31} - \frac{C_{13}}{C_{33}}e_{33}\right) + E_z^{\mathrm{AlGaN}}\frac{e_{33}^2}{C_{33}}. \tag{3}$$

It should be noted that in uncoupled analyses, the second term on the right hand side of Eq. (3) is absent.

Applying the continuity of perpendicular components of the electric displacement vector at the barrier AlGaN/GaN heterointerface, we express the field in AlGaN as follows:

$$E_z^{\mathrm{AlGaN}} = \frac{1}{\kappa^{\mathrm{AlGaN}} + (e_{33}^2/C_{33})}\left[\sigma_{\mathrm{2D}} + \Delta P^s - 2\varepsilon_x\left(e_{31} - \frac{C_{13}}{C_{33}}e_{33}\right)\right], \tag{4}$$

where κ^{AlGaN} is the permittivity of the barrier AlGaN layer and $\Delta P^s = P_{\mathrm{GaN}}^s - P_{\mathrm{AlGaN}}^s$ is the difference between the spontaneous polarization between GaN and AlGaN. The derivation of the Eq. (4) is based upon the assumption that the unintentional doping concentration of GaN is negligible. This assumption allows us to relate the electric displacement in GaN, at the AlGaN/GaN heterointerface, to the two dimensional electron gas (2DEG) charge density, σ_{2D}, as $\kappa^{\mathrm{GaN}}E_z^{\mathrm{GaN}} \cong \sigma_{\mathrm{2D}}$. Substituting (4) in (3) gives the piezoelectric component of total polarization in AlGaN as

$$P_{\mathrm{PE}}^{\mathrm{AlGaN}} = 2\varepsilon_x\left(e_{31} - \frac{C_{13}}{C_{33}}e_{33}\right)(1-\alpha) + \alpha(\sigma_{\mathrm{2D}} + \Delta P^s), \tag{5}$$

where $\alpha = (e_{33}^2/C_{33})/(\kappa^{\mathrm{AlGaN}} + e_{33}^2/C_{33})$ is a measure of the electromechanical coupling. Note that in the absence of electromechanical coupling $\alpha = 0$ and we revert back to the expression obtained by applying Hooke's law and piezoelectric polarization in an uncoupled way.

Figure 1 shows plots of the room temperature areal charge concentration due to piezoelectric polarization with and without electromechanical coupling for the case of negligible 2DEG concentration [$\sigma_{\mathrm{2D}} = 0$ in Eq. (5)], which would occur for a HFET gate biased below threshold. For computations we used the material constants reported in Ref. 4. The absence of electromechanical coupling results in an over estimation of the charge due to piezoelectric effect. From Eq. (5), we see that there are two factors contributing to the lower areal charge. First, the polarization due to the strain is reduced by a factor of $(1-\alpha)$. When electromechanical coupling is included, the amount of stress in the c plane of the AlGaN layer is lower, resulting in lower piezoelectric polarization. Second, the coupling of the electric field due to spontaneous polarization has the effect of further relaxing the tensile stress of the AlGaN layer, again lowering the piezoelectric polarization.

The application of gate bias greater than threshold induces a 2DEG concentration, σ_{2D}, in the channel of the HFET. From Eq. (5) it is clear that the change in σ_{2D} is accompanied by a change in the piezoelectric charge in AlGaN layer. Figure 2 shows the areal charge concentration due to the piezoelectric effect as a function of 2DEG concentration with Al mole fraction as a parameter for both the coupled and the uncoupled analyses. When electromechanical coupling is neglected, the polarization charge is independent of σ_{2D}. When coupling is included, the areal charge increases with increasing 2DEG concentration for a given Al mole fraction, moving toward the uncoupled value.

With the increasing 2DEG concentration corresponding to the applied gate bias becoming less negative, the compressive strain along the c axis in the barrier AlGaN layer increases.[5] Figure 3 shows the c-axis strain of an $Al_{0.3}Ga_{0.7}N$ barrier layer as a function of 2DEG concentration with and without the coupled electromechanical formulation. In the uncoupled formulation, the lattice is compressively strained by a constant value of 0.386%. However, with the incorporation of the electromechanical coupling, the magnitude of the strain in the barrier layer increases from 0.318% for a 2DEG concentration of 1×10^{12} cm^{-2} to 0.358% for a 2DEG concentration of 1×10^{13} cm^{-2}.

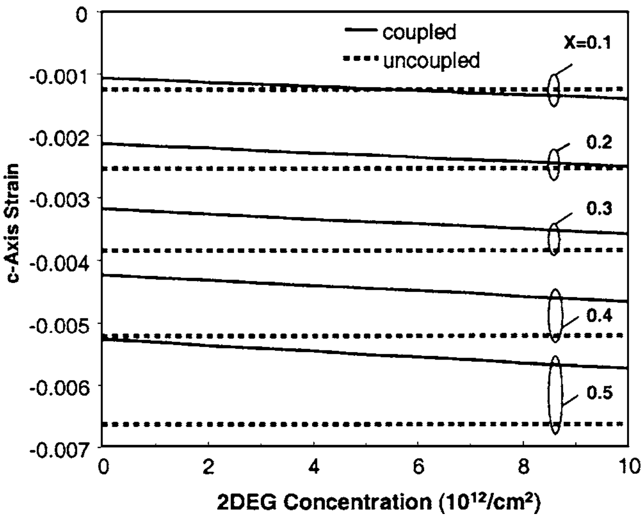

FIG. 3. Coupled strain and uncoupled strain in the *c*-axis direction of a pseudomorphic $Al_xGa_{1-x}N$ layer on GaN as a function of 2DEG concentration with aluminum mole fraction, x, as a parameter.

To account for the fact that the spontaneous and piezoelectric polarizations produce dipoles with inherently balanced charges, we have implicitly assumed the presence of surface and substrate charges that are responsible for the 2DEG concentration. Using global charge neutrality, the 2DEG concentration can be expressed as the difference of the surface and substrate charge concentrations allowing us to recast Eq. (5) in the following form:

$$P_{\mathrm{PE}}^{\mathrm{AlGaN}} = 2\varepsilon_x\left(e_{31} - \frac{C_{13}}{C_{33}}e_{33}\right)(1-\alpha) + \alpha(\sigma_{\mathrm{surface}} + \Delta P^s), \tag{6}$$

where we have neglected the contribution of the substrate charge. Global charge neutrality requires that any modification in the surface charge be accompanied by a matching change in the 2DEG concentration. The role of polarization is in the modification of the electric field in the AlGaN barrier layer, as shown in Fig. 2. With an increase in the positive surface charge, $P_{\mathrm{PE}}^{\mathrm{AlGaN}}$ increases with a concomitant decrease in the electric field as well as a corresponding change in the surface potential; this in turn must be consistent with the surface charge.

The 2DEG and the associated parasitic gate-source and gate-drain resistances are thus controlled by the surface charge. For example, applying surface passivation to modify the surface charge in the gate-source and gate-drain regions will alter the source and drain resistances. Modification of the surface charge in the gate-drain and gate-source regions may also occur when a negative gate bias causes electrons to be injected from the drain and source ends of the gate resulting in a decrease in the net positive surface charge in those regions.[8] This lowers the induced charge at the AlGaN/GaN heterointerface, increasing the parasitic drain and source resistances. The increase in parasitic resistances due to surface charge may be a mechanism of current collapse. As an alternative to global charge neutrality, local charge neutrality can be used to equate the 2DEG concentration to the difference in polarization charges at the AlGaN/GaN heterointerface. In this interpretation, a reduction in $P_{\mathrm{PE}}^{\mathrm{AlGaN}}$ [Eq. (6)] can attributed to the relaxation of in-plane stress in AlGaN layer, in agreement with the observations made by Simin *et al.*[9] It should be noted that the dynamics of current collapse will depend upon the type of traps and their associated trapping and detrapping time constants.

In conclusion, we have presented a coupled electromechanical formulation for the self-consistent determination of piezoelectric charge in AlGaN/GaN heterointerfaces. The uncoupled formulation overestimates the charge associated with piezoelectric polarization by overestimating the stress in the *c* plane and neglecting the field due to spontaneous polarization. Any surface modification caused by passivation or electron injection, for example, will change the carrier concentration in the neighborhood of AlGaN/GaN, thereby changing the source and drain resistances and influencing current collapse.

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